



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 9JFN / pdb_00009jfn
Title : Arginine decarboxylase in *Aspergillus oryzae* complexed with agmatine
Authors : Mikami, B.; Yasukawa, K.; Fujiwara, S.; Takita, T.; Mizutani, K.; Odagaki, Y.; Murakami, Y.
Deposited on : 2024-09-05
Resolution : 2.15 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

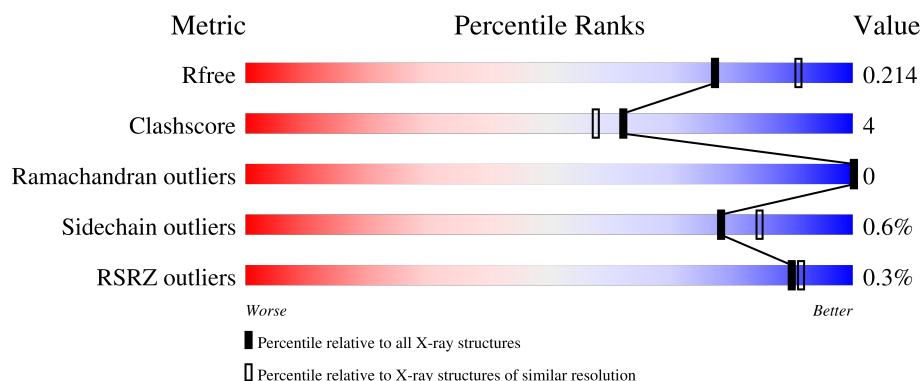
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	77% 6% 18%
1	B	462	74% 8% 18%
1	C	462	74% 9% 17%
1	D	462	75% 7% 17%
2	E	42	98% .

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Mol	Chain	Length	Quality of chain
2	F	42	 88% 12%
2	G	42	 90% 10%
2	H	42	 86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	C	501	-	-	X	-
3	PEG	C	502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15402 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	11	0
			3040	1934	515	580	11			
1	B	381	Total	C	N	O	S	0	10	0
			3031	1929	509	582	11			
1	C	382	Total	C	N	O	S	4	13	0
			3062	1950	516	585	11			
1	D	382	Total	C	N	O	S	0	9	0
			3038	1930	515	582	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q2UAM5
A	-18	GLY	-	expression tag	UNP Q2UAM5
A	-17	SER	-	expression tag	UNP Q2UAM5
A	-16	SER	-	expression tag	UNP Q2UAM5
A	-15	HIS	-	expression tag	UNP Q2UAM5
A	-14	HIS	-	expression tag	UNP Q2UAM5
A	-13	HIS	-	expression tag	UNP Q2UAM5
A	-12	HIS	-	expression tag	UNP Q2UAM5
A	-11	HIS	-	expression tag	UNP Q2UAM5
A	-10	HIS	-	expression tag	UNP Q2UAM5
A	-9	SER	-	expression tag	UNP Q2UAM5
A	-8	SER	-	expression tag	UNP Q2UAM5
A	-7	GLY	-	expression tag	UNP Q2UAM5
A	-6	LEU	-	expression tag	UNP Q2UAM5
A	-5	VAL	-	expression tag	UNP Q2UAM5
A	-4	PRO	-	expression tag	UNP Q2UAM5
A	-3	ARG	-	expression tag	UNP Q2UAM5
A	-2	GLY	-	expression tag	UNP Q2UAM5
A	-1	SER	-	expression tag	UNP Q2UAM5
A	0	HIS	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q2UAM5
B	-18	GLY	-	expression tag	UNP Q2UAM5
B	-17	SER	-	expression tag	UNP Q2UAM5
B	-16	SER	-	expression tag	UNP Q2UAM5
B	-15	HIS	-	expression tag	UNP Q2UAM5
B	-14	HIS	-	expression tag	UNP Q2UAM5
B	-13	HIS	-	expression tag	UNP Q2UAM5
B	-12	HIS	-	expression tag	UNP Q2UAM5
B	-11	HIS	-	expression tag	UNP Q2UAM5
B	-10	HIS	-	expression tag	UNP Q2UAM5
B	-9	SER	-	expression tag	UNP Q2UAM5
B	-8	SER	-	expression tag	UNP Q2UAM5
B	-7	GLY	-	expression tag	UNP Q2UAM5
B	-6	LEU	-	expression tag	UNP Q2UAM5
B	-5	VAL	-	expression tag	UNP Q2UAM5
B	-4	PRO	-	expression tag	UNP Q2UAM5
B	-3	ARG	-	expression tag	UNP Q2UAM5
B	-2	GLY	-	expression tag	UNP Q2UAM5
B	-1	SER	-	expression tag	UNP Q2UAM5
B	0	HIS	-	expression tag	UNP Q2UAM5
C	-19	MET	-	initiating methionine	UNP Q2UAM5
C	-18	GLY	-	expression tag	UNP Q2UAM5
C	-17	SER	-	expression tag	UNP Q2UAM5
C	-16	SER	-	expression tag	UNP Q2UAM5
C	-15	HIS	-	expression tag	UNP Q2UAM5
C	-14	HIS	-	expression tag	UNP Q2UAM5
C	-13	HIS	-	expression tag	UNP Q2UAM5
C	-12	HIS	-	expression tag	UNP Q2UAM5
C	-11	HIS	-	expression tag	UNP Q2UAM5
C	-10	HIS	-	expression tag	UNP Q2UAM5
C	-9	SER	-	expression tag	UNP Q2UAM5
C	-8	SER	-	expression tag	UNP Q2UAM5
C	-7	GLY	-	expression tag	UNP Q2UAM5
C	-6	LEU	-	expression tag	UNP Q2UAM5
C	-5	VAL	-	expression tag	UNP Q2UAM5
C	-4	PRO	-	expression tag	UNP Q2UAM5
C	-3	ARG	-	expression tag	UNP Q2UAM5
C	-2	GLY	-	expression tag	UNP Q2UAM5
C	-1	SER	-	expression tag	UNP Q2UAM5
C	0	HIS	-	expression tag	UNP Q2UAM5
D	-19	MET	-	initiating methionine	UNP Q2UAM5
D	-18	GLY	-	expression tag	UNP Q2UAM5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	expression tag	UNP Q2UAM5
D	-16	SER	-	expression tag	UNP Q2UAM5
D	-15	HIS	-	expression tag	UNP Q2UAM5
D	-14	HIS	-	expression tag	UNP Q2UAM5
D	-13	HIS	-	expression tag	UNP Q2UAM5
D	-12	HIS	-	expression tag	UNP Q2UAM5
D	-11	HIS	-	expression tag	UNP Q2UAM5
D	-10	HIS	-	expression tag	UNP Q2UAM5
D	-9	SER	-	expression tag	UNP Q2UAM5
D	-8	SER	-	expression tag	UNP Q2UAM5
D	-7	GLY	-	expression tag	UNP Q2UAM5
D	-6	LEU	-	expression tag	UNP Q2UAM5
D	-5	VAL	-	expression tag	UNP Q2UAM5
D	-4	PRO	-	expression tag	UNP Q2UAM5
D	-3	ARG	-	expression tag	UNP Q2UAM5
D	-2	GLY	-	expression tag	UNP Q2UAM5
D	-1	SER	-	expression tag	UNP Q2UAM5
D	0	HIS	-	expression tag	UNP Q2UAM5

- Molecule 2 is a protein called L-tryptophan decarboxylase PsiD-like domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			
2	F	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			
2	G	42	Total	C	N	O	S	0	0	0
			327	211	55	60	1			
2	H	42	Total	C	N	O	S	0	1	0
			333	215	55	62	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	502	PYR	-	modified residue	UNP Q2UAM5
F	502	PYR	-	modified residue	UNP Q2UAM5
G	502	PYR	-	modified residue	UNP Q2UAM5
H	502	PYR	-	modified residue	UNP Q2UAM5

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	F	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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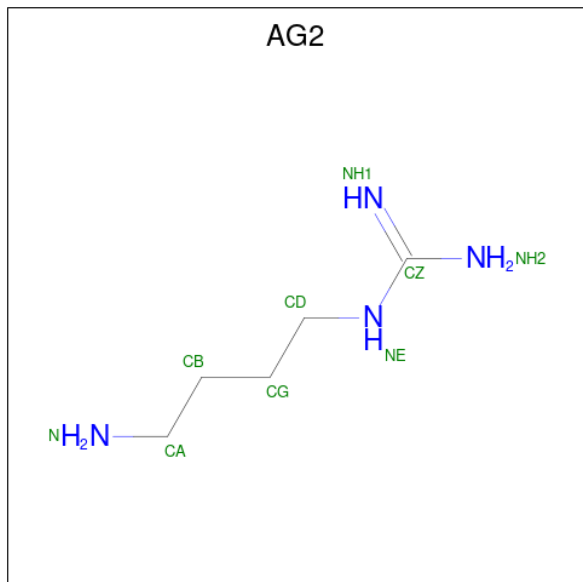
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is AGMATINE (CCD ID: AG2) (formula: $C_5H_{14}N_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	N	0	0
			9	5	4		
5	F	1	Total	C	N	0	0
			9	5	4		
5	G	1	Total	C	N	0	0
			9	5	4		
5	H	1	Total	C	N	0	0
			9	5	4		

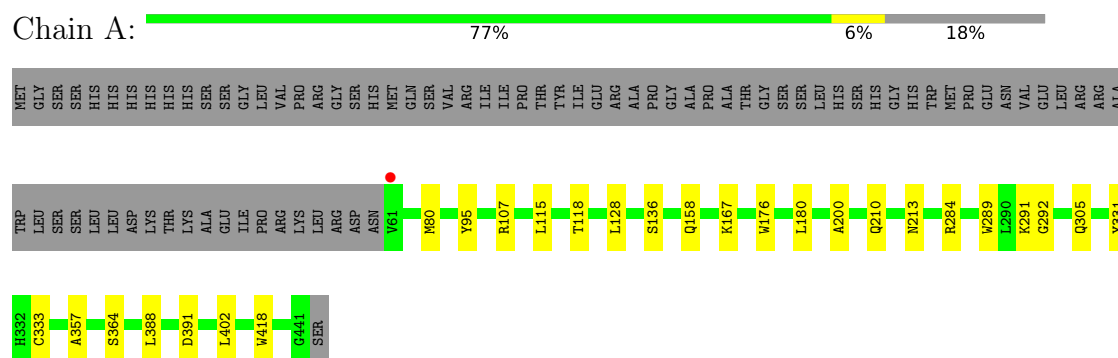
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	336	Total 336	O 336	0	0
6	E	30	Total 30	O 30	0	0
6	B	311	Total 311	O 311	0	0
6	F	30	Total 30	O 30	0	0
6	C	302	Total 302	O 302	0	0
6	G	19	Total 19	O 19	0	0
6	D	267	Total 267	O 267	0	0
6	H	22	Total 22	O 22	0	0

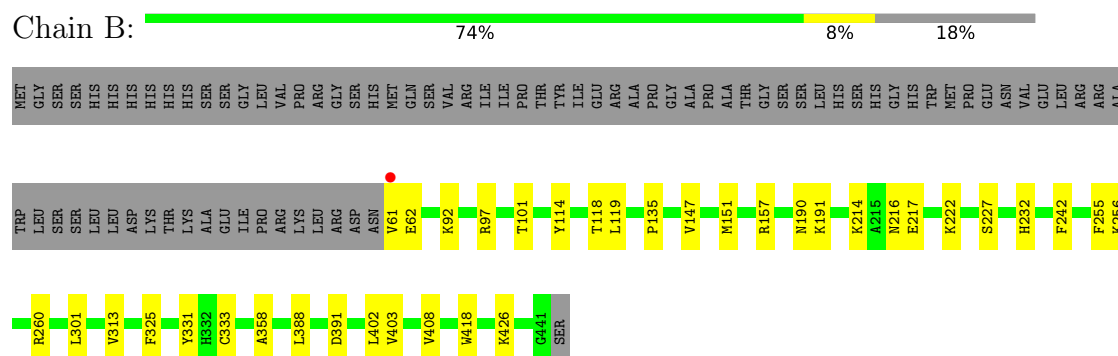
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

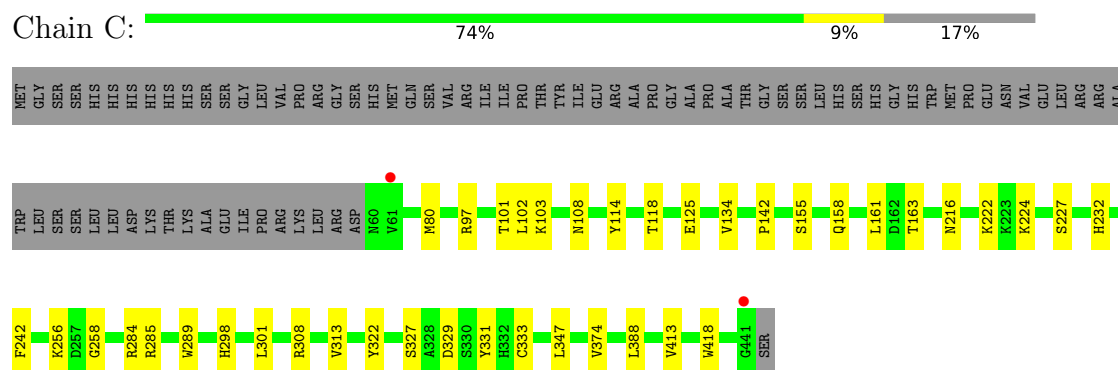
- Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein



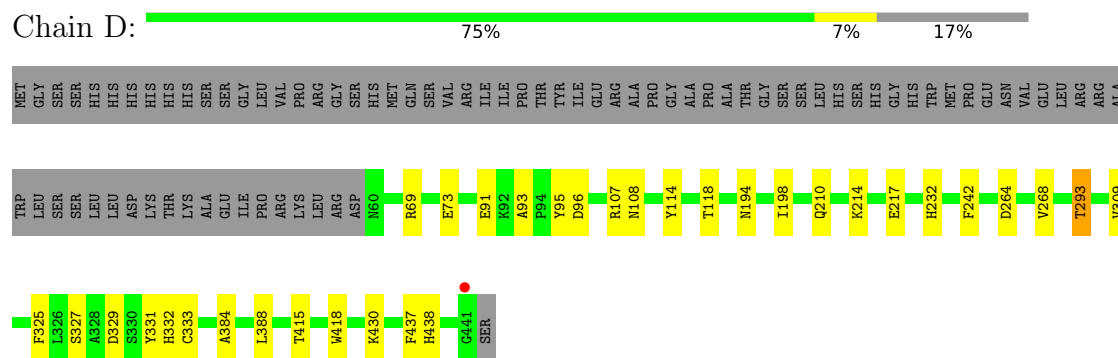
- Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein



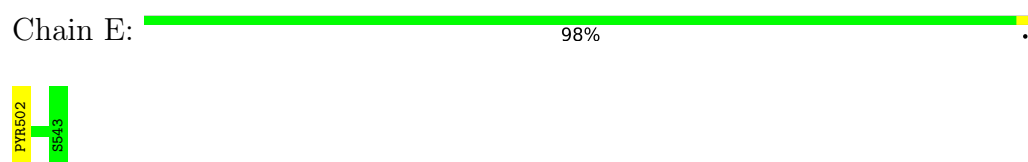
- Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein



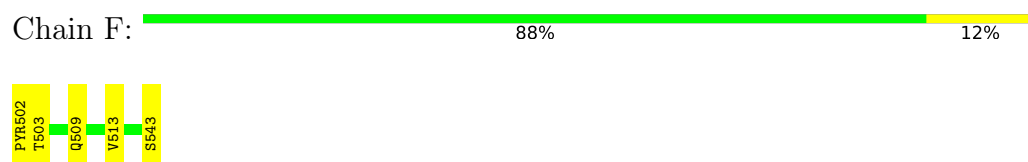
- Molecule 1: L-tryptophan decarboxylase PsiD-like domain-containing protein



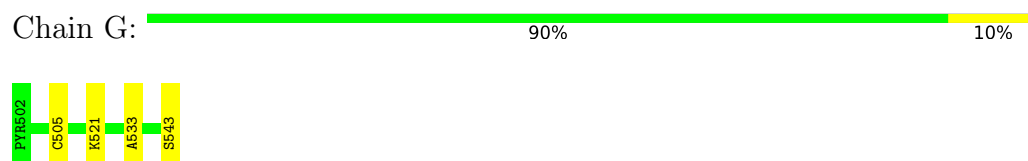
- Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein



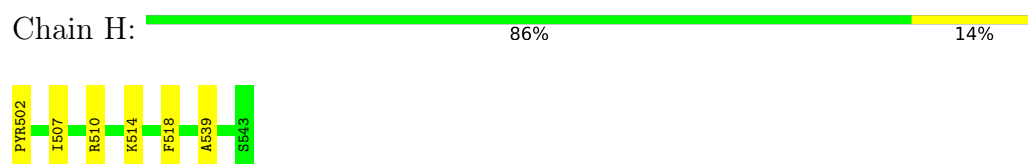
- Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein



- Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein



- Molecule 2: L-tryptophan decarboxylase PsiD-like domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	133.75Å 197.29Å 196.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.49 – 2.15 43.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.49-2.15) 99.7 (43.49-2.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.176 , 0.213 0.177 , 0.214	Depositor DCC
R_{free} test set	7002 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15402	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYR, AG2, EDO, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/3152	0.46	0/4282
1	B	0.27	0/3139	0.46	0/4264
1	C	0.28	0/3177	0.46	0/4314
1	D	0.27	0/3141	0.44	0/4270
2	E	0.25	0/337	0.48	0/456
2	F	0.25	0/337	0.44	0/456
2	G	0.26	0/328	0.48	0/444
2	H	0.24	0/337	0.40	0/456
All	All	0.27	0/13948	0.45	0/18942

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	1
2	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	502	PYR	Mainchain
2	F	502	PYR	Mainchain

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Continued from previous page...

Mol	Chain	Res	Type	Group
2	H	502	PYR	Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3040	0	2938	24	0
1	B	3031	0	2925	25	0
1	C	3062	0	2962	33	0
1	D	3038	0	2922	24	0
2	E	333	0	345	0	0
2	F	333	0	345	2	0
2	G	327	0	339	3	0
2	H	333	0	345	2	0
3	A	7	0	10	1	0
3	B	35	0	50	5	0
3	C	14	0	20	7	0
4	A	148	0	222	13	0
4	B	96	0	144	6	0
4	C	124	0	186	11	0
4	D	108	0	162	10	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
4	G	8	0	12	2	0
4	H	4	0	6	1	0
5	E	9	0	12	0	0
5	F	9	0	12	0	0
5	G	9	0	12	0	0
5	H	9	0	12	0	0
6	A	336	0	0	2	0
6	B	311	0	0	3	0
6	C	302	0	0	0	0
6	D	267	0	0	2	0
6	E	30	0	0	0	0
6	F	30	0	0	0	0
6	G	19	0	0	0	0
6	H	22	0	0	0	0
All	All	15402	0	13993	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ALA:H	4:A:517:EDO:H11	1.52	0.75
1:D:264:ASP:HA	4:D:522:EDO:H11	1.69	0.73
1:C:125:GLU:HB3	3:C:501:PEG:H31	1.71	0.71
1:D:384:ALA:HB1	4:D:525:EDO:H12	1.72	0.70
1:C:308:ARG:HH21	4:C:532:EDO:H22	1.57	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/462 (84%)	382 (98%)	8 (2%)	0	100	100
1	B	389/462 (84%)	382 (98%)	7 (2%)	0	100	100
1	C	393/462 (85%)	378 (96%)	15 (4%)	0	100	100
1	D	389/462 (84%)	378 (97%)	11 (3%)	0	100	100
2	E	41/42 (98%)	40 (98%)	1 (2%)	0	100	100
2	F	41/42 (98%)	40 (98%)	1 (2%)	0	100	100
2	G	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
2	H	41/42 (98%)	41 (100%)	0	0	100	100
All	All	1724/2016 (86%)	1679 (97%)	45 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/389 (85%)	330 (100%)	0	100	100
1	B	329/389 (85%)	328 (100%)	1 (0%)	86	91
1	C	333/389 (86%)	333 (100%)	0	100	100
1	D	329/389 (85%)	325 (99%)	4 (1%)	63	70
2	E	37/36 (103%)	37 (100%)	0	100	100
2	F	37/36 (103%)	36 (97%)	1 (3%)	39	41
2	G	36/36 (100%)	35 (97%)	1 (3%)	38	40
2	H	37/36 (103%)	35 (95%)	2 (5%)	20	16
All	All	1468/1700 (86%)	1459 (99%)	9 (1%)	78	84

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	507	ILE
2	H	514	LYS
1	D	91	GLU
1	D	293[A]	THR
1	D	293[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	531	ASN
2	G	531	ASN
1	B	332	HIS
1	B	194	ASN
2	F	523	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

136 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	D	506	-	3,3,3	0.28	0	2,2,2	0.20	0
4	EDO	A	513	-	3,3,3	0.22	0	2,2,2	0.43	0
4	EDO	C	528	-	3,3,3	0.25	0	2,2,2	0.32	0
4	EDO	C	517	-	3,3,3	0.25	0	2,2,2	0.46	0
4	EDO	C	521	-	3,3,3	0.21	0	2,2,2	0.41	0
4	EDO	B	511	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	A	526	-	3,3,3	0.25	0	2,2,2	0.30	0
4	EDO	A	537	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	C	525	-	3,3,3	0.28	0	2,2,2	0.32	0
4	EDO	B	514	-	3,3,3	0.20	0	2,2,2	0.54	0
4	EDO	B	521	-	3,3,3	0.25	0	2,2,2	0.29	0
4	EDO	C	506	-	3,3,3	0.28	0	2,2,2	0.09	0
4	EDO	C	524	-	3,3,3	0.26	0	2,2,2	0.14	0
4	EDO	A	532	-	3,3,3	0.25	0	2,2,2	0.25	0
4	EDO	D	521	-	3,3,3	0.26	0	2,2,2	0.28	0
4	EDO	A	522	-	3,3,3	0.30	0	2,2,2	0.09	0
4	EDO	C	523	-	3,3,3	0.31	0	2,2,2	0.07	0
4	EDO	D	514	-	3,3,3	0.23	0	2,2,2	0.39	0
4	EDO	A	510	-	3,3,3	0.24	0	2,2,2	0.23	0
4	EDO	C	504	-	3,3,3	0.25	0	2,2,2	0.08	0
3	PEG	C	501	-	6,6,6	0.31	0	5,5,5	0.45	0
4	EDO	C	505	-	3,3,3	0.25	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	511	-	3,3,3	0.33	0	2,2,2	0.19	0
5	AG2	F	601	2	8,8,8	0.66	0	7,8,8	0.51	0
4	EDO	D	527	-	3,3,3	0.27	0	2,2,2	0.36	0
4	EDO	A	521	-	3,3,3	0.26	0	2,2,2	0.22	0
4	EDO	A	535	-	3,3,3	0.30	0	2,2,2	0.31	0
4	EDO	C	508	-	3,3,3	0.24	0	2,2,2	0.32	0
4	EDO	C	533	-	3,3,3	0.24	0	2,2,2	0.43	0
3	PEG	A	501	-	6,6,6	0.31	0	5,5,5	0.27	0
4	EDO	A	503	-	3,3,3	0.28	0	2,2,2	0.30	0
4	EDO	B	516	-	3,3,3	0.29	0	2,2,2	0.21	0
4	EDO	E	602	-	3,3,3	0.27	0	2,2,2	0.10	0
4	EDO	D	508	-	3,3,3	0.26	0	2,2,2	0.47	0
4	EDO	A	519	-	3,3,3	0.29	0	2,2,2	0.29	0
4	EDO	D	512	-	3,3,3	0.26	0	2,2,2	0.12	0
4	EDO	D	504	-	3,3,3	0.26	0	2,2,2	0.19	0
4	EDO	C	513	-	3,3,3	0.26	0	2,2,2	0.16	0
4	EDO	B	518	-	3,3,3	0.27	0	2,2,2	0.31	0
4	EDO	C	511	-	3,3,3	0.24	0	2,2,2	0.44	0
4	EDO	C	509	-	3,3,3	0.29	0	2,2,2	0.16	0
4	EDO	A	530	-	3,3,3	0.33	0	2,2,2	0.16	0
4	EDO	D	507	-	3,3,3	0.27	0	2,2,2	0.21	0
4	EDO	A	504	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	A	536	-	3,3,3	0.26	0	2,2,2	0.34	0
4	EDO	A	523	-	3,3,3	0.28	0	2,2,2	0.59	0
4	EDO	B	509	-	3,3,3	0.26	0	2,2,2	0.26	0
4	EDO	D	511	-	3,3,3	0.26	0	2,2,2	0.29	0
3	PEG	C	502	-	6,6,6	0.28	0	5,5,5	0.51	0
4	EDO	D	509	-	3,3,3	0.27	0	2,2,2	0.23	0
4	EDO	A	508	-	3,3,3	0.28	0	2,2,2	0.29	0
4	EDO	B	515	-	3,3,3	0.27	0	2,2,2	0.12	0
4	EDO	D	502	-	3,3,3	0.24	0	2,2,2	0.45	0
4	EDO	B	513	-	3,3,3	0.28	0	2,2,2	0.20	0
4	EDO	B	510	-	3,3,3	0.24	0	2,2,2	0.40	0
4	EDO	A	531	-	3,3,3	0.29	0	2,2,2	0.16	0
4	EDO	B	506	-	3,3,3	0.27	0	2,2,2	0.16	0
4	EDO	B	507	-	3,3,3	0.26	0	2,2,2	0.24	0
4	EDO	A	509	-	3,3,3	0.24	0	2,2,2	0.49	0
4	EDO	A	502	-	3,3,3	0.17	0	2,2,2	0.30	0
5	AG2	E	601	2	8,8,8	0.61	0	7,8,8	0.48	0
4	EDO	C	530	-	3,3,3	0.25	0	2,2,2	0.21	0
4	EDO	B	529	-	3,3,3	0.27	0	2,2,2	0.27	0
4	EDO	C	515	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	A	528	-	3,3,3	0.19	0	2,2,2	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	510	-	3,3,3	0.23	0	2,2,2	0.14	0
4	EDO	C	519	-	3,3,3	0.29	0	2,2,2	0.45	0
4	EDO	A	507	-	3,3,3	0.34	0	2,2,2	0.21	0
4	EDO	A	514	-	3,3,3	0.25	0	2,2,2	0.21	0
4	EDO	D	516	-	3,3,3	0.25	0	2,2,2	0.30	0
4	EDO	B	519	-	3,3,3	0.24	0	2,2,2	0.47	0
4	EDO	A	533	-	3,3,3	0.28	0	2,2,2	0.16	0
4	EDO	D	515	-	3,3,3	0.26	0	2,2,2	0.34	0
3	PEG	B	501	-	6,6,6	0.22	0	5,5,5	0.26	0
4	EDO	D	510	-	3,3,3	0.20	0	2,2,2	0.40	0
4	EDO	B	527	-	3,3,3	0.26	0	2,2,2	0.30	0
3	PEG	B	505	-	6,6,6	0.26	0	5,5,5	0.23	0
4	EDO	C	507	-	3,3,3	0.27	0	2,2,2	0.18	0
4	EDO	A	534	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	G	603	-	3,3,3	0.30	0	2,2,2	0.27	0
4	EDO	C	516	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	B	508	-	3,3,3	0.20	0	2,2,2	0.57	0
4	EDO	A	520	-	3,3,3	0.25	0	2,2,2	0.39	0
4	EDO	B	512	-	3,3,3	0.27	0	2,2,2	0.09	0
4	EDO	A	505	-	3,3,3	0.24	0	2,2,2	0.43	0
4	EDO	C	526	-	3,3,3	0.27	0	2,2,2	0.28	0
4	EDO	B	517	-	3,3,3	0.20	0	2,2,2	0.92	0
3	PEG	B	504	-	6,6,6	0.28	0	5,5,5	0.50	0
4	EDO	B	525	-	3,3,3	0.30	0	2,2,2	0.46	0
4	EDO	D	522	-	3,3,3	0.24	0	2,2,2	0.29	0
4	EDO	A	516	-	3,3,3	0.27	0	2,2,2	0.29	0
4	EDO	D	520	-	3,3,3	0.26	0	2,2,2	0.27	0
4	EDO	D	519	-	3,3,3	0.27	0	2,2,2	0.26	0
4	EDO	F	602	-	3,3,3	0.29	0	2,2,2	0.25	0
4	EDO	A	517	-	3,3,3	0.25	0	2,2,2	0.59	0
4	EDO	C	529	-	3,3,3	0.28	0	2,2,2	0.52	0
4	EDO	C	512	-	3,3,3	0.27	0	2,2,2	0.51	0
4	EDO	C	520	-	3,3,3	0.25	0	2,2,2	0.34	0
4	EDO	A	525	-	3,3,3	0.32	0	2,2,2	0.22	0
3	PEG	B	502	-	6,6,6	0.20	0	5,5,5	0.42	0
4	EDO	C	518	-	3,3,3	0.31	0	2,2,2	0.21	0
4	EDO	A	518	-	3,3,3	0.27	0	2,2,2	0.33	0
4	EDO	D	524	-	3,3,3	0.28	0	2,2,2	0.26	0
4	EDO	B	520	-	3,3,3	0.24	0	2,2,2	0.46	0
4	EDO	A	538	-	3,3,3	0.26	0	2,2,2	0.36	0
3	PEG	B	503	-	6,6,6	0.26	0	5,5,5	0.24	0
4	EDO	H	602	-	3,3,3	0.25	0	2,2,2	0.27	0
4	EDO	C	503	-	3,3,3	0.32	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	532	-	3,3,3	0.22	0	2,2,2	0.35	0
4	EDO	D	517	-	3,3,3	0.27	0	2,2,2	0.22	0
4	EDO	D	526	-	3,3,3	0.23	0	2,2,2	0.37	0
4	EDO	D	501	-	3,3,3	0.26	0	2,2,2	0.26	0
4	EDO	D	525	-	3,3,3	0.20	0	2,2,2	0.33	0
4	EDO	D	503	-	3,3,3	0.24	0	2,2,2	0.31	0
5	AG2	H	601	2	8,8,8	0.56	0	7,8,8	0.39	0
4	EDO	D	523	-	3,3,3	0.23	0	2,2,2	0.38	0
4	EDO	B	524	-	3,3,3	0.30	0	2,2,2	0.21	0
4	EDO	B	523	-	3,3,3	0.23	0	2,2,2	0.30	0
4	EDO	A	512	-	3,3,3	0.24	0	2,2,2	0.28	0
4	EDO	A	529	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	C	527	-	3,3,3	0.31	0	2,2,2	0.15	0
4	EDO	D	505	-	3,3,3	0.29	0	2,2,2	0.32	0
4	EDO	D	513	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	A	506	-	3,3,3	0.24	0	2,2,2	0.34	0
4	EDO	A	524	-	3,3,3	0.28	0	2,2,2	0.23	0
4	EDO	C	514	-	3,3,3	0.29	0	2,2,2	0.12	0
4	EDO	D	518	-	3,3,3	0.23	0	2,2,2	0.41	0
4	EDO	A	527	-	3,3,3	0.25	0	2,2,2	0.36	0
4	EDO	C	531	-	3,3,3	0.27	0	2,2,2	0.24	0
4	EDO	G	602	-	3,3,3	0.32	0	2,2,2	0.28	0
5	AG2	G	601	2	8,8,8	0.62	0	7,8,8	0.50	0
4	EDO	C	522	-	3,3,3	0.26	0	2,2,2	0.15	0
4	EDO	B	528	-	3,3,3	0.27	0	2,2,2	0.23	0
4	EDO	B	522	-	3,3,3	0.24	0	2,2,2	0.26	0
4	EDO	A	515	-	3,3,3	0.25	0	2,2,2	0.35	0
4	EDO	B	526	-	3,3,3	0.22	0	2,2,2	0.82	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	506	-	-	0/1/1/1	-
4	EDO	A	513	-	-	1/1/1/1	-
4	EDO	C	528	-	-	1/1/1/1	-
4	EDO	C	517	-	-	1/1/1/1	-
4	EDO	C	521	-	-	0/1/1/1	-
4	EDO	B	511	-	-	1/1/1/1	-
4	EDO	A	526	-	-	0/1/1/1	-
4	EDO	A	537	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	525	-	-	0/1/1/1	-
4	EDO	B	514	-	-	0/1/1/1	-
4	EDO	B	521	-	-	1/1/1/1	-
4	EDO	C	506	-	-	0/1/1/1	-
4	EDO	C	524	-	-	0/1/1/1	-
4	EDO	A	532	-	-	0/1/1/1	-
4	EDO	D	521	-	-	1/1/1/1	-
4	EDO	A	522	-	-	0/1/1/1	-
4	EDO	C	523	-	-	1/1/1/1	-
4	EDO	D	514	-	-	0/1/1/1	-
4	EDO	A	510	-	-	0/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
3	PEG	C	501	-	-	2/4/4/4	-
4	EDO	C	505	-	-	0/1/1/1	-
4	EDO	A	511	-	-	0/1/1/1	-
5	AG2	F	601	2	-	0/6/6/6	-
4	EDO	D	527	-	-	1/1/1/1	-
4	EDO	A	521	-	-	0/1/1/1	-
4	EDO	A	535	-	-	0/1/1/1	-
4	EDO	C	508	-	-	0/1/1/1	-
4	EDO	C	533	-	-	0/1/1/1	-
3	PEG	A	501	-	-	2/4/4/4	-
4	EDO	A	503	-	-	0/1/1/1	-
4	EDO	B	516	-	-	1/1/1/1	-
4	EDO	E	602	-	-	1/1/1/1	-
4	EDO	D	508	-	-	0/1/1/1	-
4	EDO	A	519	-	-	1/1/1/1	-
4	EDO	D	512	-	-	0/1/1/1	-
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	C	513	-	-	0/1/1/1	-
4	EDO	B	518	-	-	0/1/1/1	-
4	EDO	C	511	-	-	0/1/1/1	-
4	EDO	C	509	-	-	0/1/1/1	-
4	EDO	A	530	-	-	1/1/1/1	-
4	EDO	D	507	-	-	0/1/1/1	-
4	EDO	A	504	-	-	1/1/1/1	-
4	EDO	A	536	-	-	0/1/1/1	-
4	EDO	A	523	-	-	1/1/1/1	-
4	EDO	B	509	-	-	1/1/1/1	-
4	EDO	D	511	-	-	0/1/1/1	-
3	PEG	C	502	-	-	3/4/4/4	-
4	EDO	D	509	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	508	-	-	0/1/1/1	-
4	EDO	B	515	-	-	0/1/1/1	-
4	EDO	D	502	-	-	1/1/1/1	-
4	EDO	B	513	-	-	0/1/1/1	-
4	EDO	B	510	-	-	1/1/1/1	-
4	EDO	A	531	-	-	1/1/1/1	-
4	EDO	B	506	-	-	0/1/1/1	-
4	EDO	B	507	-	-	0/1/1/1	-
4	EDO	A	509	-	-	0/1/1/1	-
4	EDO	A	502	-	-	0/1/1/1	-
5	AG2	E	601	2	-	0/6/6/6	-
4	EDO	C	530	-	-	1/1/1/1	-
4	EDO	B	529	-	-	0/1/1/1	-
4	EDO	C	515	-	-	0/1/1/1	-
4	EDO	A	528	-	-	0/1/1/1	-
4	EDO	C	510	-	-	0/1/1/1	-
4	EDO	C	519	-	-	1/1/1/1	-
4	EDO	A	507	-	-	1/1/1/1	-
4	EDO	A	514	-	-	0/1/1/1	-
4	EDO	D	516	-	-	0/1/1/1	-
4	EDO	B	519	-	-	1/1/1/1	-
4	EDO	A	533	-	-	1/1/1/1	-
4	EDO	D	515	-	-	0/1/1/1	-
3	PEG	B	501	-	-	1/4/4/4	-
4	EDO	D	510	-	-	0/1/1/1	-
4	EDO	B	527	-	-	0/1/1/1	-
3	PEG	B	505	-	-	1/4/4/4	-
4	EDO	C	507	-	-	0/1/1/1	-
4	EDO	A	534	-	-	0/1/1/1	-
4	EDO	G	603	-	-	0/1/1/1	-
4	EDO	C	516	-	-	0/1/1/1	-
4	EDO	B	508	-	-	0/1/1/1	-
4	EDO	A	520	-	-	0/1/1/1	-
4	EDO	B	512	-	-	1/1/1/1	-
4	EDO	A	505	-	-	0/1/1/1	-
4	EDO	C	526	-	-	0/1/1/1	-
4	EDO	B	517	-	-	1/1/1/1	-
3	PEG	B	504	-	-	2/4/4/4	-
4	EDO	B	525	-	-	1/1/1/1	-
4	EDO	D	522	-	-	1/1/1/1	-
4	EDO	A	516	-	-	0/1/1/1	-
4	EDO	D	520	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	519	-	-	0/1/1/1	-
4	EDO	F	602	-	-	1/1/1/1	-
4	EDO	A	517	-	-	0/1/1/1	-
4	EDO	C	529	-	-	0/1/1/1	-
4	EDO	C	512	-	-	0/1/1/1	-
4	EDO	C	520	-	-	0/1/1/1	-
4	EDO	A	525	-	-	1/1/1/1	-
3	PEG	B	502	-	-	2/4/4/4	-
4	EDO	C	518	-	-	1/1/1/1	-
4	EDO	A	518	-	-	1/1/1/1	-
4	EDO	D	524	-	-	0/1/1/1	-
4	EDO	B	520	-	-	0/1/1/1	-
4	EDO	A	538	-	-	0/1/1/1	-
3	PEG	B	503	-	-	1/4/4/4	-
4	EDO	H	602	-	-	0/1/1/1	-
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	C	532	-	-	0/1/1/1	-
4	EDO	D	517	-	-	0/1/1/1	-
4	EDO	D	526	-	-	0/1/1/1	-
4	EDO	D	501	-	-	0/1/1/1	-
4	EDO	D	525	-	-	0/1/1/1	-
4	EDO	D	503	-	-	0/1/1/1	-
5	AG2	H	601	2	-	0/6/6/6	-
4	EDO	D	523	-	-	1/1/1/1	-
4	EDO	B	524	-	-	1/1/1/1	-
4	EDO	B	523	-	-	1/1/1/1	-
4	EDO	A	512	-	-	1/1/1/1	-
4	EDO	A	529	-	-	0/1/1/1	-
4	EDO	C	527	-	-	0/1/1/1	-
4	EDO	D	505	-	-	0/1/1/1	-
4	EDO	D	513	-	-	1/1/1/1	-
4	EDO	A	506	-	-	1/1/1/1	-
4	EDO	A	524	-	-	0/1/1/1	-
4	EDO	C	514	-	-	1/1/1/1	-
4	EDO	D	518	-	-	0/1/1/1	-
4	EDO	A	527	-	-	0/1/1/1	-
4	EDO	C	531	-	-	1/1/1/1	-
4	EDO	G	602	-	-	1/1/1/1	-
5	AG2	G	601	2	-	0/6/6/6	-
4	EDO	C	522	-	-	1/1/1/1	-
4	EDO	B	528	-	-	1/1/1/1	-
4	EDO	B	522	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	515	-	-	1/1/1/1	-
4	EDO	B	526	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 61 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	PEG	O1-C1-C2-O2
3	A	501	PEG	O2-C3-C4-O4
3	C	501	PEG	O2-C3-C4-O4
3	B	502	PEG	O1-C1-C2-O2
3	C	502	PEG	O2-C3-C4-O4

There are no ring outliers.

41 monomers are involved in 56 short contacts:

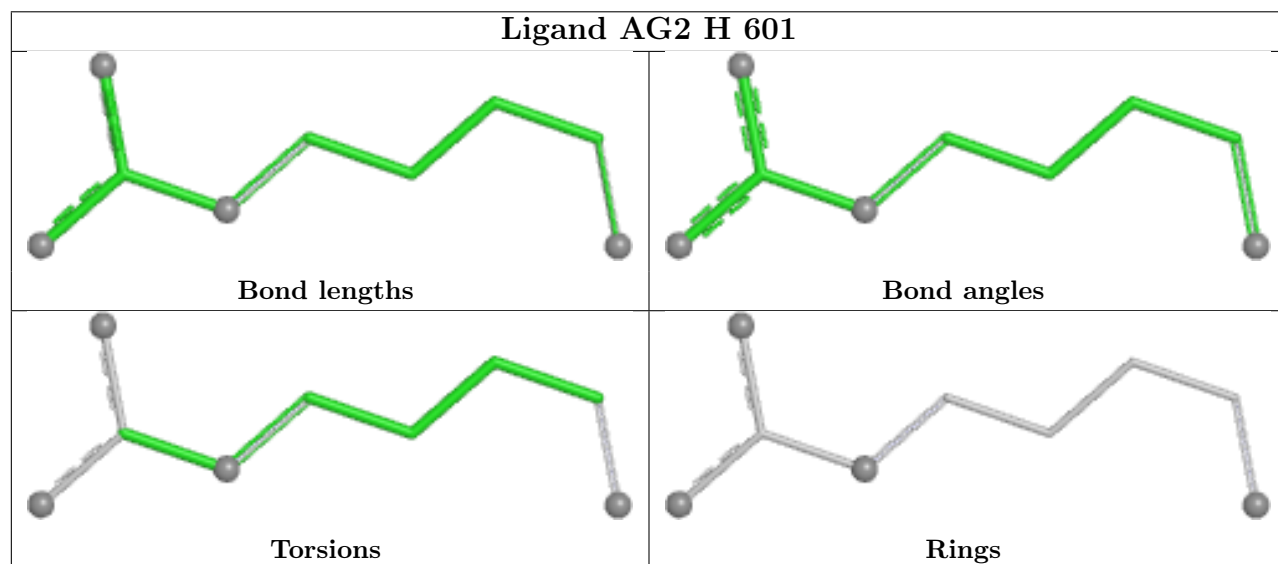
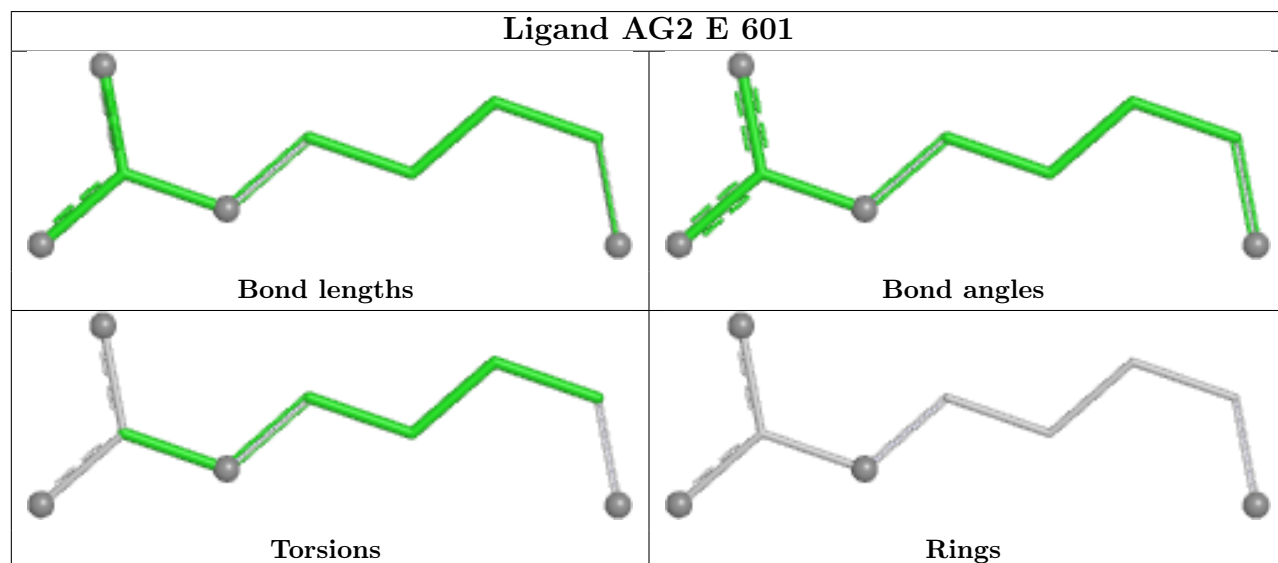
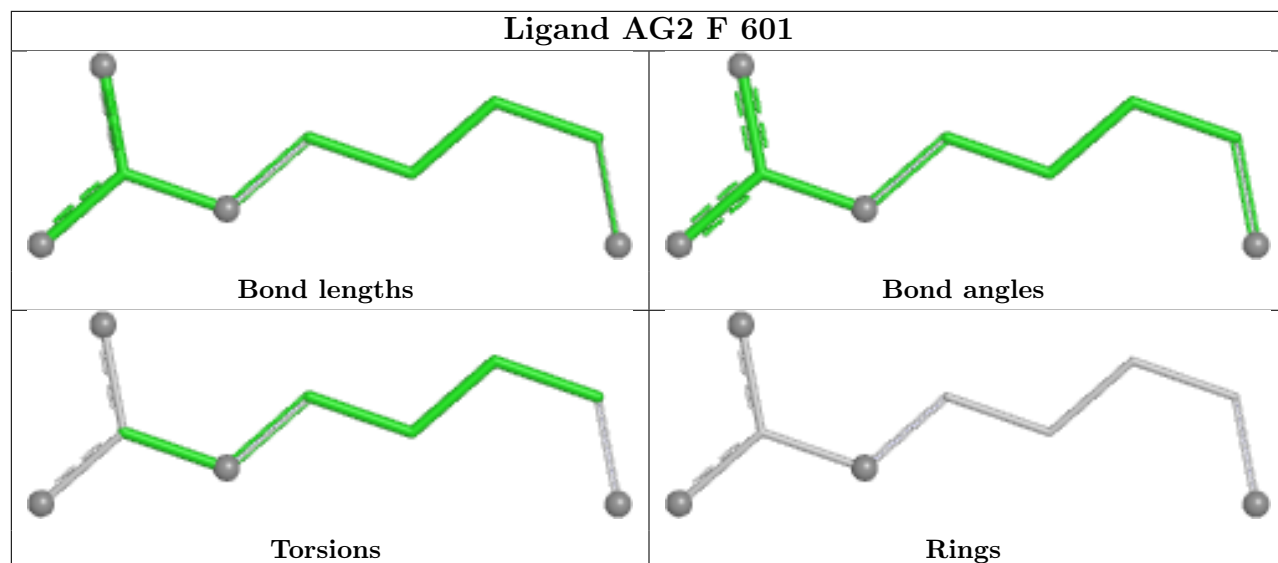
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	528	EDO	1	0
4	A	526	EDO	1	0
4	C	525	EDO	2	0
4	B	514	EDO	1	0
4	B	521	EDO	2	0
4	C	524	EDO	1	0
4	D	514	EDO	1	0
4	A	510	EDO	1	0
3	C	501	PEG	4	0
4	D	527	EDO	1	0
3	A	501	PEG	1	0
4	D	504	EDO	1	0
4	A	530	EDO	2	0
3	C	502	PEG	4	0
4	C	530	EDO	2	0
4	B	529	EDO	1	0
4	A	514	EDO	1	0
4	A	533	EDO	2	0
3	B	501	PEG	2	0
4	A	534	EDO	1	0
4	G	603	EDO	1	0
3	B	504	PEG	1	0

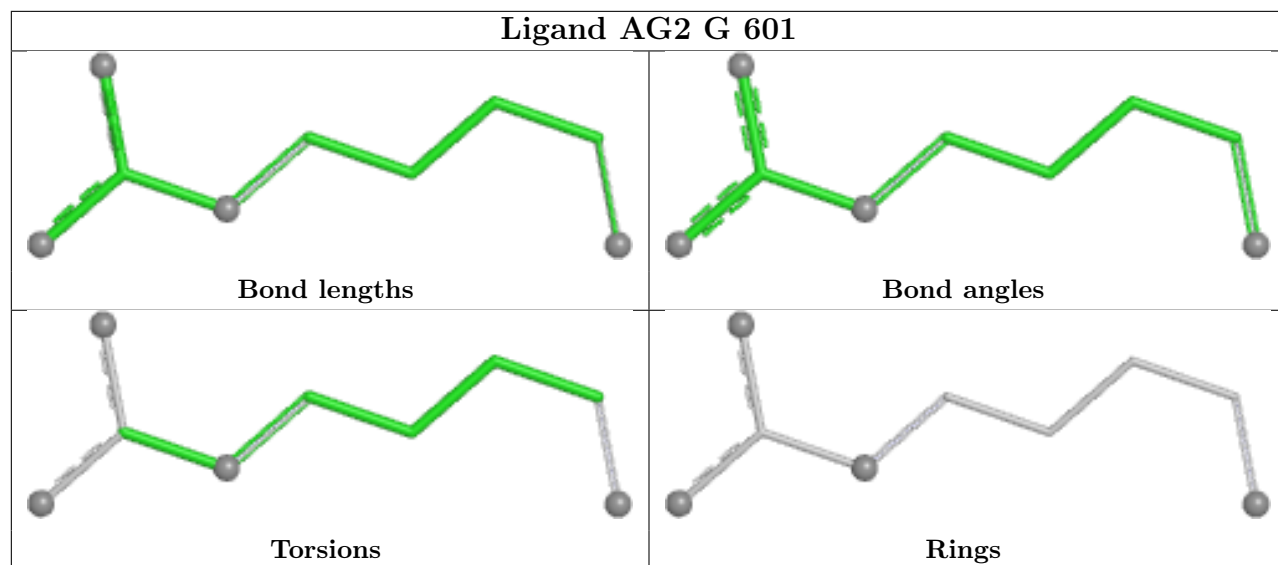
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	525	EDO	1	0
4	D	522	EDO	2	0
4	D	520	EDO	1	0
4	A	517	EDO	1	0
4	C	512	EDO	1	0
4	C	520	EDO	1	0
3	B	502	PEG	2	0
4	C	518	EDO	1	0
4	A	518	EDO	2	0
4	H	602	EDO	1	0
4	C	532	EDO	2	0
4	D	525	EDO	1	0
4	B	523	EDO	1	0
4	A	512	EDO	1	0
4	C	527	EDO	1	0
4	D	505	EDO	1	0
4	D	513	EDO	2	0
4	G	602	EDO	1	0
4	A	515	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	381/462 (82%)	-0.39	1 (0%) 90 91	18, 37, 49, 80	11 (2%)
1	B	381/462 (82%)	-0.28	1 (0%) 90 91	18, 37, 57, 77	10 (2%)
1	C	382/462 (82%)	-0.15	2 (0%) 87 89	18, 39, 54, 97	13 (3%)
1	D	382/462 (82%)	-0.08	1 (0%) 90 91	18, 41, 62, 105	9 (2%)
2	E	41/42 (97%)	-0.27	0 100 100	20, 37, 56, 81	1 (2%)
2	F	41/42 (97%)	-0.28	0 100 100	22, 41, 57, 80	1 (2%)
2	G	41/42 (97%)	0.01	0 100 100	32, 40, 61, 77	0
2	H	41/42 (97%)	-0.05	0 100 100	22, 43, 55, 83	1 (2%)
All	All	1690/2016 (83%)	-0.22	5 (0%) 90 91	18, 39, 57, 105	46 (2%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	61	VAL	3.4
1	B	61	VAL	2.9
1	D	441	GLY	2.5
1	C	441	GLY	2.5
1	C	61	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	D	524	4/4	0.66	0.23	60,67,71,72	0
3	PEG	C	502	7/7	0.67	0.23	47,59,63,65	0
4	EDO	B	514	4/4	0.69	0.17	61,61,61,77	0
4	EDO	D	511	4/4	0.70	0.13	69,71,75,77	0
4	EDO	B	523	4/4	0.71	0.26	61,63,67,81	0
4	EDO	D	516	4/4	0.72	0.14	70,78,80,82	0
4	EDO	A	524	4/4	0.72	0.16	58,64,66,67	0
4	EDO	D	509	4/4	0.73	0.19	55,56,60,62	0
3	PEG	B	505	7/7	0.74	0.17	60,64,66,71	0
4	EDO	B	515	4/4	0.74	0.16	66,68,71,72	0
4	EDO	A	530	4/4	0.74	0.23	51,52,57,57	0
4	EDO	G	602	4/4	0.74	0.20	45,62,63,73	0
4	EDO	A	531	4/4	0.75	0.16	56,57,61,78	0
4	EDO	A	512	4/4	0.76	0.25	47,59,63,68	0
4	EDO	A	535	4/4	0.77	0.20	47,53,56,60	0
4	EDO	B	519	4/4	0.77	0.18	64,65,66,76	0
4	EDO	B	521	4/4	0.77	0.15	56,62,64,70	0
4	EDO	C	531	4/4	0.78	0.18	58,61,62,62	0
4	EDO	A	511	4/4	0.78	0.23	36,50,52,54	0
4	EDO	C	510	4/4	0.79	0.25	43,55,60,62	0
4	EDO	D	521	4/4	0.79	0.14	67,71,76,80	0
4	EDO	C	517	4/4	0.79	0.22	55,59,67,67	0
4	EDO	B	525	4/4	0.80	0.18	33,48,61,62	0
4	EDO	C	523	4/4	0.80	0.18	61,61,64,68	0
4	EDO	A	515	4/4	0.80	0.21	50,51,58,66	0
4	EDO	D	515	4/4	0.81	0.13	68,74,76,81	0
4	EDO	B	524	4/4	0.81	0.16	49,50,55,57	0
4	EDO	A	519	4/4	0.81	0.18	42,47,52,56	0
3	PEG	A	501	7/7	0.81	0.18	32,51,59,61	0
4	EDO	D	520	4/4	0.82	0.14	64,65,67,69	0
4	EDO	C	504	4/4	0.82	0.20	49,51,53,59	0
4	EDO	A	523	4/4	0.82	0.13	45,52,58,59	0
4	EDO	D	526	4/4	0.82	0.15	59,59,63,75	0
4	EDO	A	529	4/4	0.83	0.20	56,60,65,69	0
4	EDO	G	603	4/4	0.83	0.18	47,53,57,58	0
4	EDO	A	513	4/4	0.83	0.15	48,53,55,72	0
4	EDO	D	522	4/4	0.83	0.13	59,66,69,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	528	4/4	0.83	0.17	41,53,53,57	0
4	EDO	A	525	4/4	0.83	0.20	48,54,56,66	0
4	EDO	A	538	4/4	0.84	0.15	55,63,66,71	0
4	EDO	C	527	4/4	0.84	0.20	51,54,58,58	0
4	EDO	A	522	4/4	0.84	0.19	55,57,57,59	0
4	EDO	A	532	4/4	0.84	0.18	47,52,57,61	0
4	EDO	A	509	4/4	0.84	0.15	44,46,52,62	0
4	EDO	D	506	4/4	0.84	0.12	66,70,71,76	0
4	EDO	C	522	4/4	0.84	0.21	53,61,61,67	0
4	EDO	D	510	4/4	0.84	0.17	46,53,55,60	0
4	EDO	D	512	4/4	0.85	0.18	55,58,64,65	0
4	EDO	C	511	4/4	0.85	0.16	39,43,48,52	0
4	EDO	C	524	4/4	0.85	0.17	54,60,62,64	0
4	EDO	D	503	4/4	0.85	0.17	58,60,63,78	0
3	PEG	B	501	7/7	0.85	0.18	50,55,62,75	0
4	EDO	C	530	4/4	0.85	0.16	41,53,54,58	0
4	EDO	D	523	4/4	0.85	0.12	45,57,58,64	0
4	EDO	B	511	4/4	0.85	0.17	52,52,63,66	0
4	EDO	D	525	4/4	0.85	0.17	46,51,53,58	0
4	EDO	C	533	4/4	0.85	0.13	46,50,56,62	0
4	EDO	H	602	4/4	0.85	0.15	54,58,59,75	0
4	EDO	A	527	4/4	0.86	0.12	58,62,66,68	0
4	EDO	C	507	4/4	0.86	0.16	47,47,55,63	0
4	EDO	A	528	4/4	0.86	0.13	40,48,51,58	0
4	EDO	C	525	4/4	0.86	0.14	46,50,61,62	0
4	EDO	C	526	4/4	0.86	0.17	51,61,62,65	0
3	PEG	B	504	7/7	0.86	0.11	32,43,51,54	0
4	EDO	C	514	4/4	0.86	0.14	65,70,72,78	0
4	EDO	C	516	4/4	0.86	0.13	63,64,67,70	0
4	EDO	B	513	4/4	0.86	0.15	57,64,73,75	0
3	PEG	B	502	7/7	0.87	0.13	38,48,56,62	0
4	EDO	A	521	4/4	0.87	0.16	64,68,69,77	0
4	EDO	D	517	4/4	0.87	0.16	64,68,69,71	0
4	EDO	D	519	4/4	0.87	0.14	52,55,59,67	0
4	EDO	A	510	4/4	0.87	0.18	54,59,59,59	0
4	EDO	C	515	4/4	0.87	0.14	61,63,64,65	0
4	EDO	D	505	4/4	0.87	0.14	41,45,56,56	0
4	EDO	B	512	4/4	0.87	0.19	51,55,59,67	0
4	EDO	A	533	4/4	0.87	0.22	53,54,59,67	0
4	EDO	C	529	4/4	0.87	0.17	43,49,52,62	0
4	EDO	C	518	4/4	0.87	0.17	49,60,61,65	0
4	EDO	C	520	4/4	0.87	0.19	53,58,61,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	E	602	4/4	0.88	0.18	57,60,61,67	0
4	EDO	B	508	4/4	0.88	0.14	48,49,63,65	0
3	PEG	B	503	7/7	0.88	0.12	64,67,75,75	0
4	EDO	A	514	4/4	0.88	0.12	54,55,62,72	0
4	EDO	C	532	4/4	0.88	0.10	46,51,58,60	0
4	EDO	D	527	4/4	0.88	0.15	44,48,49,57	0
4	EDO	D	514	4/4	0.88	0.13	48,52,55,63	0
4	EDO	B	516	4/4	0.89	0.18	56,58,62,67	0
4	EDO	D	513	4/4	0.89	0.13	51,53,63,65	0
4	EDO	A	534	4/4	0.90	0.09	54,57,57,65	0
4	EDO	B	526	4/4	0.90	0.11	42,45,49,51	0
4	EDO	C	519	4/4	0.90	0.17	45,50,57,58	0
4	EDO	C	528	4/4	0.90	0.27	44,47,49,55	0
3	PEG	C	501	7/7	0.90	0.13	38,44,60,66	0
4	EDO	A	520	4/4	0.90	0.13	56,60,62,68	0
4	EDO	C	505	4/4	0.90	0.13	46,47,56,69	0
4	EDO	D	518	4/4	0.90	0.13	42,44,46,56	0
4	EDO	C	506	4/4	0.90	0.14	53,54,56,64	0
4	EDO	A	526	4/4	0.91	0.11	46,53,59,64	0
4	EDO	D	504	4/4	0.91	0.11	43,46,53,63	0
4	EDO	A	506	4/4	0.91	0.13	41,44,47,59	0
4	EDO	B	520	4/4	0.91	0.15	54,57,60,64	0
4	EDO	D	508	4/4	0.91	0.13	44,48,52,53	0
4	EDO	B	510	4/4	0.92	0.10	44,47,47,58	0
4	EDO	B	517	4/4	0.92	0.13	43,47,50,50	0
4	EDO	B	527	4/4	0.92	0.13	42,49,57,62	0
4	EDO	B	518	4/4	0.92	0.12	49,51,54,56	0
4	EDO	B	529	4/4	0.92	0.12	47,48,54,59	0
4	EDO	F	602	4/4	0.92	0.11	43,45,45,55	0
4	EDO	A	508	4/4	0.92	0.13	45,51,54,60	0
4	EDO	A	537	4/4	0.92	0.09	49,49,54,55	0
4	EDO	C	521	4/4	0.92	0.14	49,57,59,66	0
4	EDO	A	505	4/4	0.92	0.11	39,39,51,51	0
4	EDO	A	516	4/4	0.92	0.10	41,52,54,63	0
4	EDO	A	517	4/4	0.92	0.13	36,39,45,55	0
4	EDO	C	512	4/4	0.93	0.12	51,55,57,70	0
4	EDO	C	509	4/4	0.93	0.08	45,45,46,53	0
4	EDO	A	504	4/4	0.93	0.10	40,43,51,57	0
4	EDO	D	507	4/4	0.93	0.14	61,67,70,76	0
4	EDO	B	522	4/4	0.93	0.17	46,58,58,60	0
4	EDO	B	509	4/4	0.94	0.12	51,51,54,56	0
4	EDO	A	507	4/4	0.94	0.12	39,47,52,57	0

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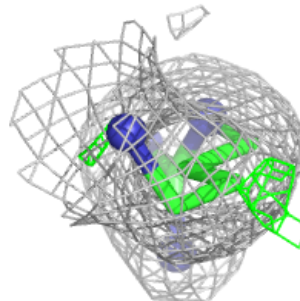
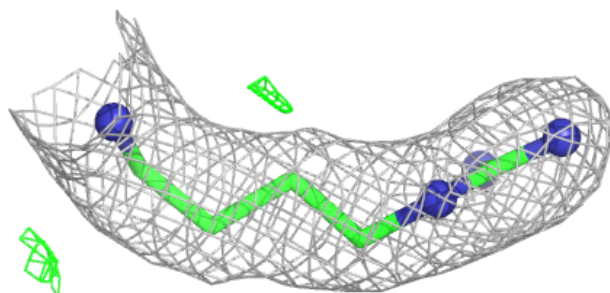
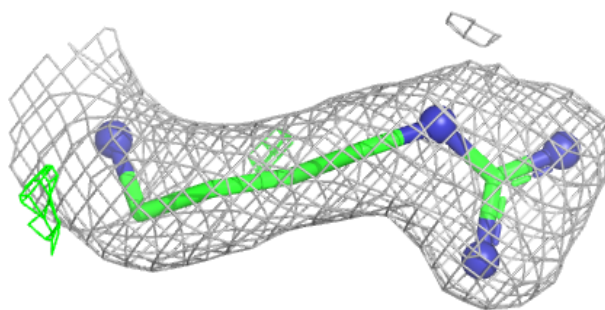
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	536	4/4	0.94	0.12	38,61,65,68	0
4	EDO	B	507	4/4	0.94	0.10	39,40,41,42	0
4	EDO	A	518	4/4	0.94	0.16	44,47,48,48	0
4	EDO	C	513	4/4	0.94	0.15	44,48,58,61	0
4	EDO	A	502	4/4	0.95	0.07	29,33,34,34	0
4	EDO	D	502	4/4	0.95	0.09	42,45,47,47	0
5	AG2	E	601	9/9	0.95	0.07	30,32,40,41	0
5	AG2	F	601	9/9	0.95	0.08	31,35,36,39	0
5	AG2	G	601	9/9	0.95	0.08	34,36,43,45	0
5	AG2	H	601	9/9	0.95	0.08	34,39,43,47	0
4	EDO	C	503	4/4	0.96	0.07	31,32,33,38	0
4	EDO	D	501	4/4	0.96	0.07	35,36,37,40	0
4	EDO	C	508	4/4	0.96	0.09	43,46,51,53	0
4	EDO	B	506	4/4	0.97	0.07	34,35,40,41	0
4	EDO	A	503	4/4	0.97	0.08	38,43,43,44	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

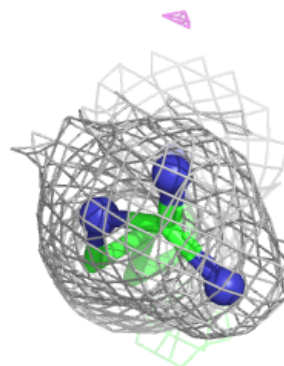
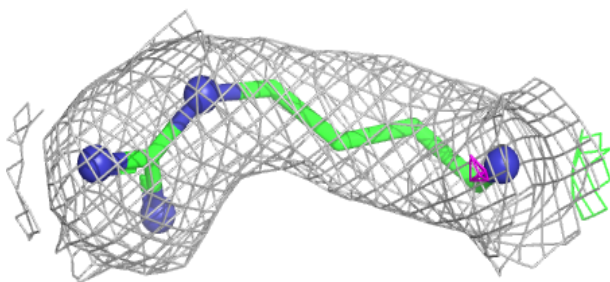
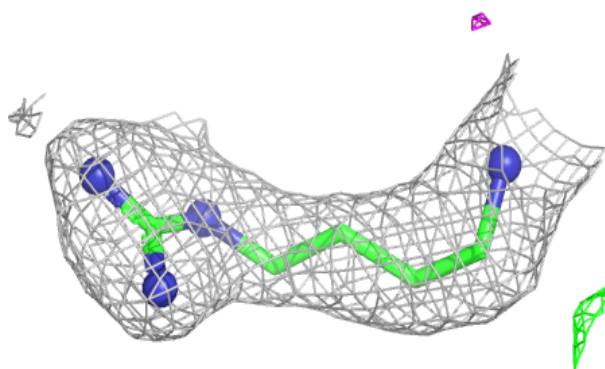
Electron density around AG2 E 601:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

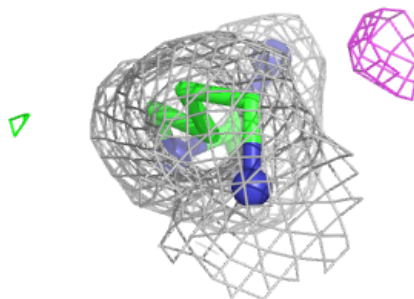
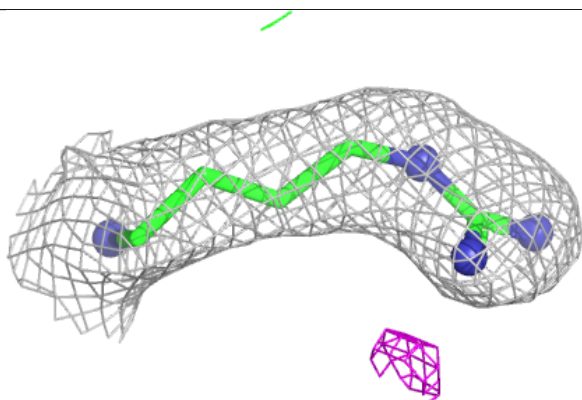
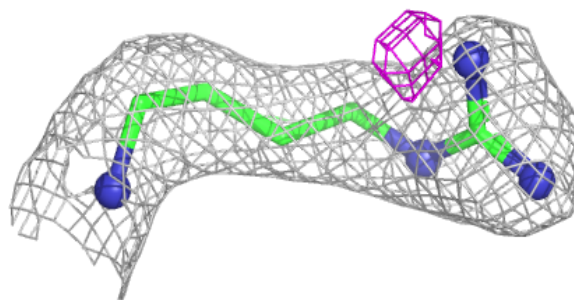


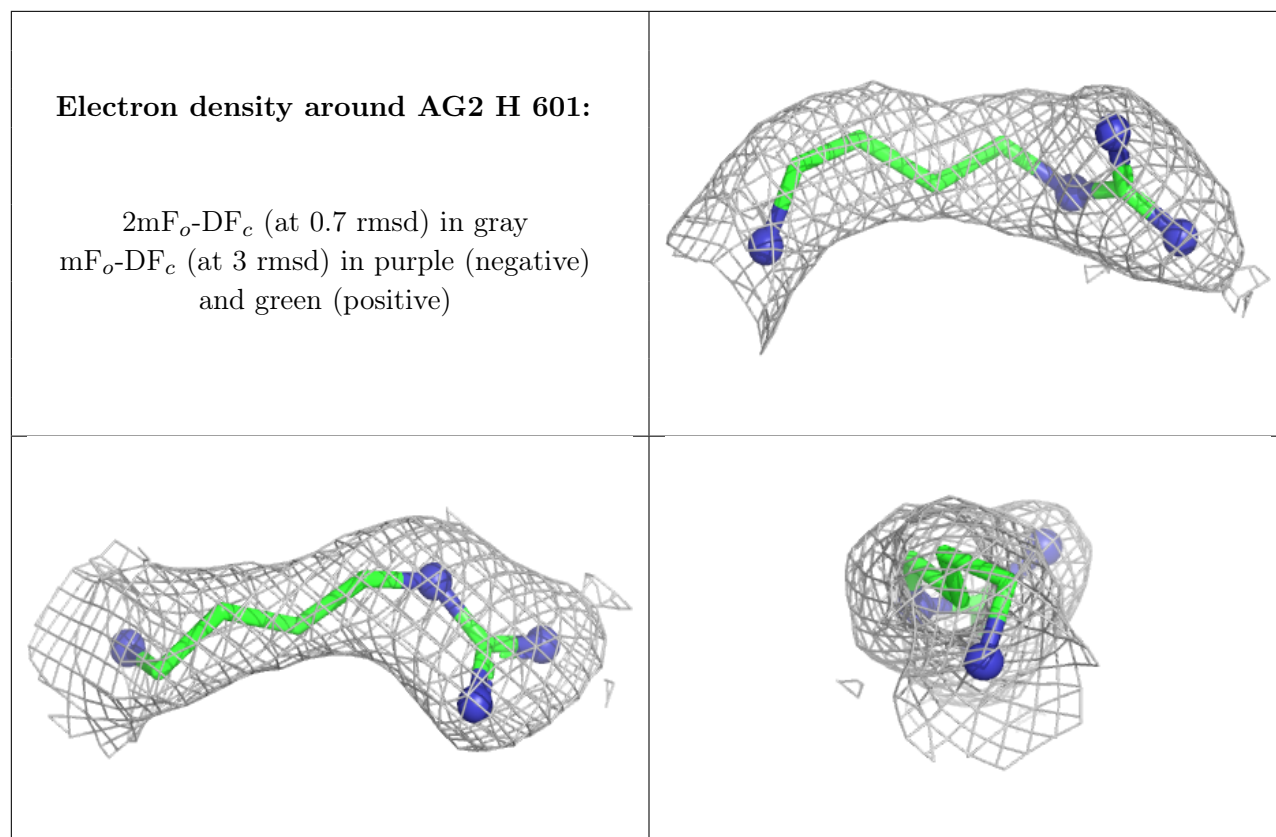
Electron density around AG2 F 601:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around AG2 G 601:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.